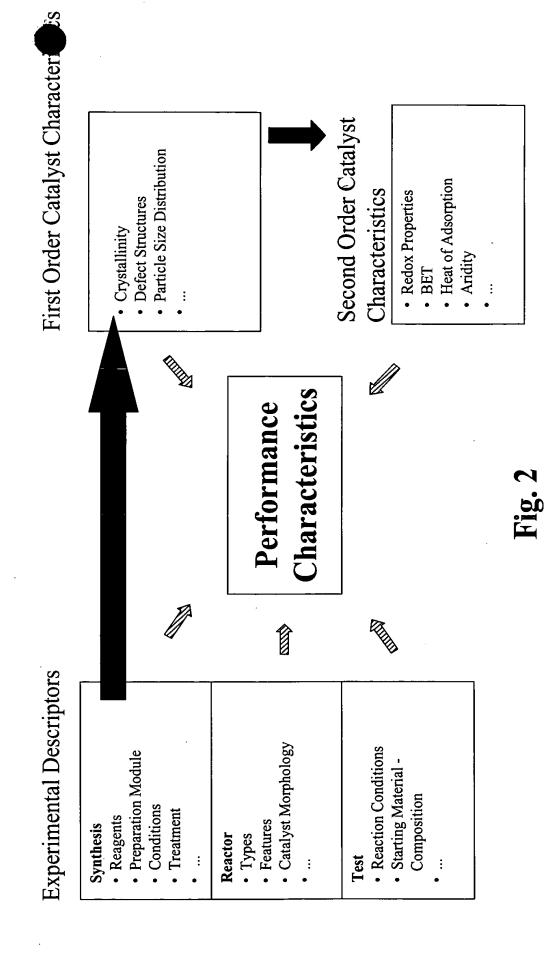


LIBRARIES

Inventor(s): Dr. Stephen A. SCHUNK Dr. John M. NEWSAM DOCKET NO.: 078096/0105

Sheet 2 of 9 sheets Figs 1-7 RPEET/TJBURNS

Performance Characteristics



<u>ogerale nenga</u>

RPEET/TJBURNS

Initial Substance Library Operator

Library Design New Plausibility Testing Evolutionary ' Algorithms Correlations Statistics Database Production Analysis Testing Operator

Manual Support

RPEET/TJBURNS Analysis & **DATA EVALUATION** Samples Test Raw Material Store Sample Archive Sample details Data Flow and Material Flow Test FILE SERVER DATABASE Statistics/Data Mining Evolutionary Algorithms Analysis n Chemicals, Solutions, Mixtures Analysis 2 Post-Treatment Synthesis Analysis Feedback for Amended Test Parameters Feedback for Amended Library Design

Title: COMPUTER-AIDED OPTIMIZATION OF SUBSTANCE
LIBRARIES
Inventor(s): Dr. Stephen A. SCHUN
Dr. John M. NEWSAM
DOCKET NO.: 078096/0105
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Title: COMPUTER-AIDED OPTIMIZATION OF SUBSTANCE LIBRARIES

Inventor(s): Dr. Stephen A. SCHO.
Dr. John M. NEWSAM
DOCKET NO.: 078096/0105
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RPEET/TJBURNS

Original Library Design and Tests Using the Entire Parameter Space

Step 2: Data Acquisition

Step 1: Design of Library, Test and Process Conditions

Feed C₁ Support oxide

Precursor Reduction Oxidation

Hd

Reynolds

Heat Exchange

	Experiment 1	Experiment 2	Experiment n
Τ			
р		6. C. T.	
Feed	254,648		
ر ا			
'ئ		BXYX	
Support oxide			
PH			
Precursor	NEW YORK		
Reduction			
Oxidation			
Reynolds			
Heat	Manager.		Salar S
Exchange			

‡	•
+	‡
#	+
Activity	Selectivity

Fig. 5a

TANCE

LIBRARIES Inventor(s): Dr. Stephen A. SCHUNK Dr. John M. NEWSAM DOCKET NO.: 078096/0105

OMPUTER-AIDED OPTIMIZATION OF

Sheet 6 of 9 sheets Figs 1-7

RPEET/TJBURNS

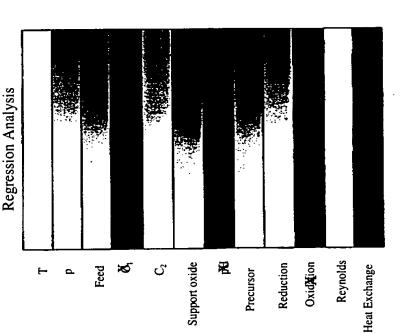
Regression Analysis, Energies of the Parameter Space

Step 3: Evaluation of the Significant of the Design and Test Parameters

Confirmation of Trends Step 4: Test of the Regression Analysis

the Library, Test and Process Step 5: Amended Design of

Conditions



Principle of Genetic Algorithms

Title: COMPUTER-AIDED OPTIMIZATION OF SUBSTANCE LIBRARIES

Inventor(s): Dr. Stephen A. SCHUNK Dr. John M. NEWSAM DOCKET NO.: 078096/0105 Sheet 7 of 9 sheets Figs 1-7

RPEET/TJBURNS

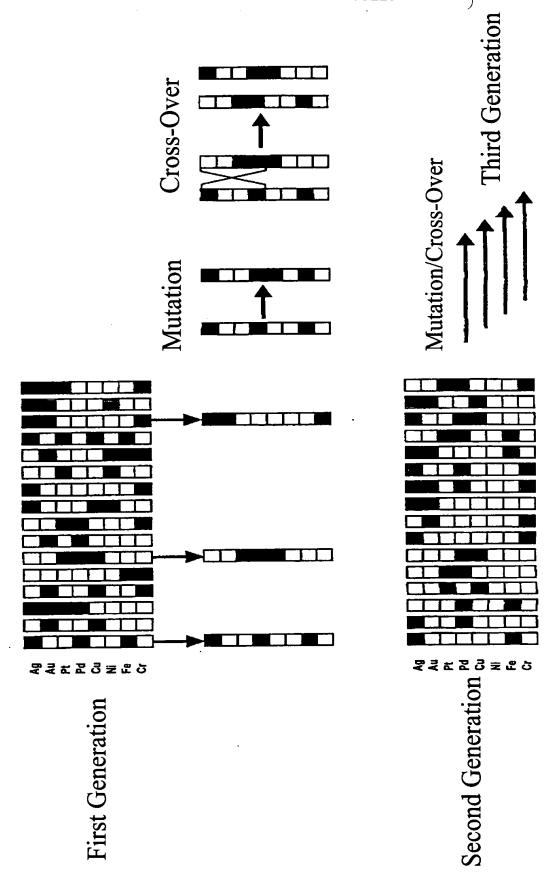


Fig. 5c

Title: COMPUTER-AIDED OPTIMIZATION OF SUBSTANCE LIBRARIES

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RPEET/TJBURNS

Sensitivity Analysis of the Parameters of the Initial Library Pareto Diagram

Pareto Chart of Standardized Effects; Variable: U_NOX 7 factors, 5 Blocks, 96 Runs; MS Residual=128,2875

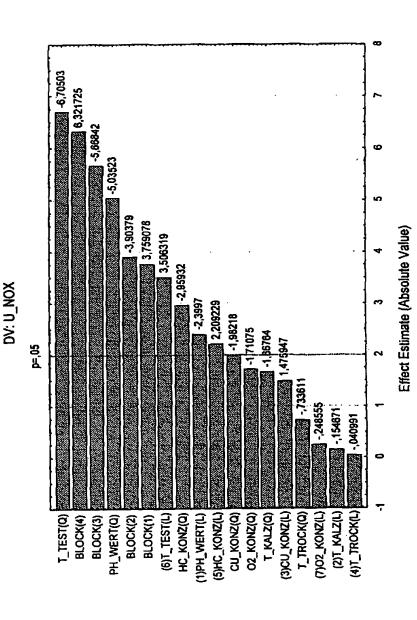


Fig. 6

COMPUTER-AIDED OPTIMIZATION O

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<u>.</u>

of the 1st Optimized Library Pareto Diagram Sensitivity Analysis of the Parameters

Pareto Chart of Standardized Effects; Variable: U_NOX 4 factors, 2 Blocks, 48 Runs; MS Residual=99,09295

